# SIAM Activity Group on Computational Science and Engineering Charter Renewal Application

This CHARTER RENEWAL applies to the SIAM Activity Group on Computational Science and Engineering. The SIAM Activity Group (or SIAG) to which this renewal applies was originally formed under the aegis of SIAM on December 15, 2000 by the SIAM Council and December 2, 2000 by the SIAM Board of Trustees with its initial operating period beginning January 1, 2001 and ending December 31, 2003. Its charter has been renewed by the Council and Board eleven times thereafter.

This SIAG has 2398 members, including 1074 student members, as of December 31, 2021.

According to its Rules of Procedure, the objective(s) of the SIAM Activity Group on Computational Science and Engineering are to:

- Foster collaborations among applied mathematicians, computer scientists, domain scientists and engineers in those areas of research related to the theory, development, and use of computational technologies for the solution of problems in science and engineering.
- Promote and facilitate Computational Science and Engineering as an academic discipline.
- Promote computational simulation as a peer to theory and experiment in the process of scientific discovery.

Within the framework of SIAM, the SIAG will conduct activities that implement its purposes. The SIAG on CSE will undertake a number of activities, including:

Organize minisymposia at the SIAM Annual Meeting on years where there is no SIAG conference.

- Organize a track of at least six minisymposia at the SIAM Annual Meeting at least once every seven years. The VP for Programs and the VP at Large will coordinate the scheduling with the SIAG Chair.
- 2) Organize a biennial SIAM Conference on Computational Science and Engineering. The SIAG will consider dovetailing specialized workshops and conferences with the SIAM Annual Meeting or other SIAG conferences. The Chair of the Conference Organizing Committee shall be either the Program Director or the Chair of the SIAG or their designee. The organizing committee must be approved by the VP for Programs at least 16 months before the conference.
- 3) With the approval of the SIAM Program Committee, the SIAG may organize special sessions at SIAM meetings, and conduct special one--- or two---day meetings immediately before or after a regular SIAM meeting. Other SIAG meetings may be organized only with the approval of the SIAM President and Vice President for Programs.
- 4) Broker partnerships between academia, industry, and government laboratories. The SIAG will seek to facilitate the establishment of academic programs in CSE to foster its development as an academic discipline. The SIAG also will facilitate the placement of undergraduate and graduate students in internships in industry and government laboratories.

- 5) Work with other societies to promote CSE. The SIAG will work with other professional societies to promote CSE. For example, SIAM and another society might organize a workshop on a topic of mutual interest. The SIAG also would attempt to increase government support for CSE through various outreach activities.
- 6) Disseminate information. The SIAG may publish a newsletter, offer a members' list serve or maintain a website to facilitate the exchange of information among its members and other interested parties. SIAG meetings, workshops, and conferences may be organized only with the approval of the SIAM President and the SIAM Vice President for Programs.

The SIAG has complemented SIAM's activities and supported its proposed functions. The answers to the questions below indicate how this was accomplished and what the officers propose as the future directions for the SIAG.

#### List all current officers of the activity group.

Chair: Stefan Wild

Vice Chair: Jeff Hammond Program Director: Judith Hill Secretary: Tan Bui-Thanh

# 1) How is the field covered by the activity group doing? Is it growing, is the focus shifting? What have been the significant advances over the last two years?

The field of computational science and engineering (CSE) continues to grow and play a vital role in industry, academia, and government research across the globe.

SIAM notes the following. Computational science and engineering complement theory and experiment as a critical component of scientific discovery and the third pillar of sciences. More and more universities, for example, UT Austin, MIT, Harvard, Princeton, Purdue, UIUC, GaTech, have established CSE majors, concentrations, certificates, etc. Some, including UT Austin and Virginia Tech, now have undergraduate majors in CSE. CSE is indispensable for leading-edge investigation and engineering design in a vast number of industrial sectors, including, for example, aerospace, automotive, biological, chemical, and semiconductor technologies that all rely increasingly on advanced modeling and simulation. CSE also contributes to policy and decisions relating to human health, resources, transportation, and defense. Finally, in many new areas such as medicine, the life sciences, management, and marketing (e.g., data and stream mining), and finance, techniques, and algorithms from CSE are of growing importance. CSE is naturally interdisciplinary. Its goals concern understanding and analyzing complex systems, predicting their behavior, and optimizing processes and designs. Thus, CSE grows out of its physical applications, while depending on mathematical algorithms, computer architecture and software, and having at its core, powerful algorithms. At the frontiers of CSE remain many open problems and challenges, including the verification, validation, and uncertainty quantification of computational models; the analysis and assimilation of large and complex data sets, including techniques for visualization and animation; and the design of flexible CSE software.

The role of simulation continues to expand to diverse scientific and engineering fields. The worldwide pandemic has likely increased computational research and development activities that complement experimental and observational data collection and analysis. The field continues to see a rapid uptick in developing and adopting data-driven (e.g., machine learning) techniques. Similarly, advances are being made to address the increasing heterogeneity of computing resources at all scales.

It is an exciting time for computational science and engineering. More than twenty-one countries are represented in the top 100 entries of the November 2020 Top500 Supercomputer list. Computational science and engineering is an international phenomenon.

2) How is the activity group doing? Is it remaining vibrant? Is the size of the SIAG stable or increasing? How is the SIAG keeping up with the changes in the field? How are the broader interests of SIAM reflected in the activities of the SIAG?

With 2398 members, SIAG CSE remains the largest and one of the most vibrant SIAGs in SIAM. Notably, this is a 13% decrease from the SIAG's membership (2751) two years ago. This overall decrease is due to a 25% drop in student members over the same period. The number of non-student members increased slightly in the same time frame. The SIAG still has the largest number of student members (1074), but this decline was likely due to an overall drop in SIAM student members and the emergence of new SIAGs. We hypothesize that student membership should stabilize post-pandemic with the current SIAGs but would continue to decrease when additional SIAGs are created.

Of the students, there are 245 females, 759 male, 6 non-binary, 55 not-indicated, and 9 prefer-not-to-disclose members. Of the non-students, there are 215 female, 1053 male, 2 non-binary, 38 not-indicated, and 16 prefer-not-to-disclose members.

The SIAG's biennial conference is SIAM's largest SIAG meeting. The broad interests of the SIAG are best reflected by the minisymposia submitted to its biennial conference. At <u>SIAM CSE 2021</u>, there was a strong representation of a broad array of science and engineering fields, including biology, biomechanics, chemistry, climate, energy, fluid dynamics, geophysics, materials, and medicine. Scientific computing, including numerical methods and their analysis, continued to be the core of the conference. A number of minisymposia addressed high-performance computing and emerging architectures, with an increase seen in mixed-/reduced-precision and "unreliable"/nondeterministic computing. Many minisymposia also addressed various aspects of software, from building communities to software sustainability. Data-driven techniques and applications continued to spread throughout the conference, with topics including graph-based learning, reduced-order models, and scientific machine learning.

There is strong interest in the SIAG in advancing diversity, equity, and inclusion efforts in our technical community. We particularly note strong attendance in a three-part panel discussion at CSE21 on D&I for careers in CSE. The first part had panelists share their experiences of being a minority in CSE. The second part had panelists discuss effective practices in promoting D&I. The third and final part was interactive and focused on reactions and Q&A from the panels. The <u>Broader Engagement program</u>, performed in partnership with the <u>Sustainable Horizons Institute</u> for the fourth time at CSE, engaged a record number (over 100) of participants in the new virtual format. BE participants presented 47 posters at CSE21.

3) Please list conferences/workshops the activity group has sponsored or co-sponsored over the past two years, and give a brief (one sentence or phrase) indication of the success or problems with each.

The 2021 SIAM Conference on Computational Science and Engineering was held March 1-5, 2021. Although originally scheduled for Fort Worth, TX, it shifted to 100% remote due to the Covid19 pandemic. This shift presented significant challenges for the organizing committee and SIAM. Participation remained vibrant:

• 2,511 Registered (a 32% increase over CSE19)

- 1,785 speakers and 359 minisymposia (major changes were made at CSE21, with minisymposia increased to 5 speakers and integration of all contributed talks into minisymposia; for comparison, CSE19 had 401 4-speaker minisymposia)
- 6 two-part minitutorials (solicited through an open call for the first time; over 40 submissions were received)
- 152 Travel Awards (a significant increase given that these awards only covered registration)
- 189 Poster Presenters (split across two sessions and featuring a plenary poster blitz)
- 10 Poster Awards (including 2 best student presenters and 2 best blitz presentations)
- A <u>virtual career fair</u> was held with 16 organizations joining as exhibitors; this was the first CSE conference where career fair exhibitors paid a fee to attend.
- 4) Please indicate the number of minisymposia directly organized by the activity group at the last two SIAM annual meetings. When did the SIAG last organize a track at an annual meeting or meet jointly with the SIAM Annual Meeting?

\*Because of the number of Activity Groups, the current guidelines are that an Activity Group should organize a track about every seven (7) Annual Meetings or meet jointly with the Annual Meeting within a seven (7) meeting period.\*

SIAG CSE last organized a track at the 2019 International Congress on Industrial and Applied Mathematics. The track consisted of 21 CSE-sponsored minisymposia, eight of which were multi-part sessions.

For the 2020 SIAM Annual meeting, the SIAG helped organizing committee member Hans de Sterck identify an appropriate plenary speaker representing SIAG CSE (Lars Ruthotto).

5) Please indicate other activities sponsored by the activity group, to include newsletters, prizes and web sites. Have each of these been active and successful?

The SIAG awards two prizes biennially; these were most recently awarded in 2021. The prizes are highly competitive; for example, in 2021 17 complete nomination packets were received for the SIAG CSE early career prize.

The 2021 SIAM Activity Group on Computational Science and Engineering Best Paper Prize was awarded to James Vogel, Jianlin Xia, Stephen Cauley, and Venkataramanan Balakrishnan. Their award-winning paper, "Superfast Divide-and-Conquer Method and Perturbation Analysis for Structured Eigenvalue Solution," was published originally in the SIAM Journal on Scientific Computing in 2016. The authors were recognized for impressive work, which reduces the computational complexity of a whole eigendecomposition of Hermitian matrices from cubic to loglinear by utilizing the hierarchical semi-separable structure.

The <u>2021 SIAM Activity Group on Computational Science and Engineering Early Career Prize</u> was awarded to Paris Perdikaris. Paris was recognized for his work on machine learning using Gaussian

processes and neural networks, which has set the foundation for a new paradigm in data-driven and physics-informed scientific computing.

Additionally, two other prize lectures were hosted at CSE21. George Em Karniadakis was awarded the <u>2021 SIAM/ACM Prize in Computational Science and Engineering</u>. Stefan Güttel was awarded the <u>2021 James H. Wilkinson Prize for Numerical Analysis and Scientific Computing</u>.

A February 2021 SIAM News article spotlighted these 4 prizes and the winners.

SIAG mailing lists were moved to the Engage platform in 2021. SIAG CSE almost exclusively uses <a href="Engage">Engage</a> as a mailing list. The community is very active, with over 426 SIAG CSE emails sent since Engage was established. The list receives roughly one email per day. Given this significant traffic, the SIAG's officers led a SIAM pilot to not require officer moderation for every post. This has worked out exceptionally well; currently the only emails that require moderator action are those sent by a SIAG CSE member who has never interacted with Engage (i.e., after this first moderation (anywhere on Engage), their subsequent SIAG CSE emails will not require moderation). We encourage the following types of postings to the mailing list: solicitations for SIAG CSE-sponsored conferences, announcements of CSE-related conferences/events, calls for nominations of prizes, software, open positions, and SIAM announcements such as electronic publication, general conference announcements, and other news.

Early in 2022, the SIAG set up a Twitter account at <a href="https://twitter.com/siagcse">https://twitter.com/siagcse</a>. The SIAG is also in the process of moving from a difficult-to-maintain <a href="wiki-webpage">wiki-webpage</a> to a <a href="mailto:github-based-webpage">github-based-webpage</a>.

6) What activities are planned and proposed for the next period of the charter? Please describe scheduled and suggested future activities in detail.

<u>Prizes:</u> The SIAG currently has open calls for its two aforementioned prizes. Both prizes will have presentations at CSE23. Additionally, SIAM has seemingly formalized the move of other SIAG-relevant prizes to have prize lectures at the SIAG's biennial conference. The <u>2023 James H. Wilkinson Prize for Numerical Software</u> will be awarded at CSE23. The <u>2023 SIAM/ACM Prize in Computational Science and Engineering</u> will also be awarded at CSE23. The <u>2025 James H. Wilkinson Prize for Numerical Analysis and Scientific Computing</u> will be awarded at CSE25. Formalizing these awards at CSE conferences is excellent for planning purposes and to increase the visibility of the awardees. One potential downside is that it may be more difficult for the SIAG to start new prizes (which members often inquire about, given the size of the SIAG) as more of the SIAG's conference footprint is prefilled.

Additionally, the SIAG is leading a SIAM pilot to not post prize committee composition until after the nomination window has closed. Given the large numbers of nominations the SIAG receives for its prizes, established committee members often had to step down from the committee because of a conflict of interest with a nomination. With the current change, COIs are known at the time of nomination closure, and hence the committee composition can be finalized and made public at that time.

<u>CSE Conference planning:</u> Because the CSE conference is now SIAM's largest conference, it requires significantly larger facilities and greater levels of organization than most SIAG conferences. Planning further in advance is needed to ensure availability of sufficient resources (venues, speakers, etc.) and

enable conference organizers to learn from the experiences of past conference organizers. In 2020, the SIAG shifted the conference planning activities of the CSE Program Director to focus on the conference four years ahead.

#### Specifically:

- The Program Director elected to serve from 20XY through 20XY+1 will plan the CSE conference to be held in 20XY+4 (rather than the 20XY+2 conference).
- The Program Director is expected to chair the 20XY+4 CSE Organizing Committee; an appropriate designee may be nominated by SIAG CSE officers and approved by SIAM's VP of Programs.
- The Program Director will work with SIAM to identify an appropriate venue for CSE 20XY+4 by the end of 20XY+1, propose co-chairs, assemble an organizing committee, and begin planning of CSE 20XY+4.
- The Program Director will participate as an observer in 20XY+2 CSE conference planning to learn from the experiences of the CSE 20XY+2 organizing committee.

The current Program Director (Judith Hill) will thus organize the 2025 CSE conference. Since 2023 is a transition period, the previous SIAG Chair (Karen Devine) is representing the SIAG as a co-chair at CSE23. To date, this shift has worked extremely well. The Program Director has been meeting with the CSE23 co-chairs regularly to shadow the process. We expect that this will significantly improve the institutional memory associated with organizing the CSE conference.

<u>CSE23</u> will be held February 26-March 3, 2023, in Amsterdam! Roughly one-third of the SIAG CSE membership works outside the United States, and so it is great to see CSE held outside of the United States for the first time. Karen Devine, Dirk Hartmann, and Wil Schilders are serving as co-chairs. The first CSE hackathon is being planned in conjunction with the conference. CSE23 is also emphasizing the "I" in SIAM by encouraging more industrial participation and including industry-focused activities.

With the advancing of the CSE conference schedule, timing and location for <u>CSE25</u> are already known: CSE25 will be held March 2-7, 2025, in Fort Worth, TX. The SIAG expects to announce co-chairs in the coming months with the intention that the organizing committee for CSE25 will be established before CSE23 so that these individuals can view CSE23 through the lens of future organizers.

To fairly represent non-US members and increase participation in SIAG CSE globally, the 2017-18 officers proposed a six-year rotation for location of the biennial CSE conference. The proposal specifies that the conference rotate between the eastern US, the western US, and an overseas location over three occurrences of the conference. CSE23 will be in Amsterdam, CSE25 will be in Fort Worth, Texas, and so CSE27 will be held somewhere in the United States geographically distinct from Texas. The SIAG expects that the 2023-2024 officers will solicit proposals for hosting CSE29 outside of the United States.

### 7) How can SIAM help the activity group achieve its goals?

SIAM can best help the CSE community by continuing to promote CSE through conferences, publications, and student programs. CSE methods and competence are becoming increasingly relevant for scientists in fields other than mathematics; SIAM should consider strategies to attract more members from these disciplines and integrate them under the CSE umbrella.

SIAM has a strong record of offering opportunities for leadership, service, and mentoring to under-represented populations; SIAM can help SIAGs by continuing to support programs that promote diversity in the SIAGs. The SIAG would like to see SIAM address DEI across the whole society. SIAM can also help SIAG CSE by better integrating with Broader Engagement programs popular with the SIAG. As the CSE conference grows, the support needed from SIAM grows as well. SIAM has done an excellent job with SIAG CSE's new forward-looking timetable. SIAM can help the SIAG by formalizing the SIAG's advanced planning so that future SIAG officers, CSE organizers, and SIAM staff are adequately prepared for advanced sighting and scheduling. The CSE conferences often break new ground for SIAM conferences; for example, CSE23 will feature hackathons and a robust industrial program. SIAM can help the SIAG by empowering the CSE co-chairs to innovate and explore new ways to engage the community at CSE conferences located in the United States.

The SIAG could benefit from SIAM following best practices in implementing aliases for SIAG-related emails. The SIAG would like to see SIAG-related aliases (both for the SIAG membership and for the SIAG officers) using @siam.org. Currently, SIAG officers have to set up their own channel for SIAG members and nonmembers to contact the officers, and paid SIAG members contact the SIAG using @ConnectedCommunity.org.

For prize administration, SIAM can help the SIAG by coordinating prize committees across the 2 SIAG prizes and the 3 non-SIAG prizes that the SIAG hosts at CSE. Both SIAG prizes receive relatively large pools of nominations. SIAM can help the SIAG by making the identification of conflicts of interest easier for potential committee members and by improving the interface that committee members use to access materials. For example, a popular request of SIAG award committees is to provide a single way to download all submissions and/or collate them in a single document for review.

The SIAG has a large proportion of nonacademic members. SIAM can help the SIAG by expanding its effort to engage such members and encourage greater nonacademic participation in SIAGs overall. SIAM could also help the SIAG by making web-based content more readily accessible. SIAG CSE appreciates SIAM's commitment to sustainable content, transparency, and public access. A remaining challenge is that SIAG-relevant content (e.g., to the SIAG, its conferences, its prizes, general SIAM processes for all SIAG-related functions) continues to be that archive.siam.org content is the top choice for most web indexers and that the associated pages do not clearly indicate where the up-to-date content is hosted. The current state of affairs continues to place a burden on prospective SIAG members, conference attendees, and volunteers. Although SIAM's current web content is a recognized potential for improvement, SIAGs could significantly benefit from SIAM restructuring its content such that archives are maintained while ensuring that the recent generations of content are maintained. An example of this is that all past SIAG charters are and should be indexed from a perpetually maintained common SIAM page, but a potential SIAM outsider is

encountering <a href="https://archive.siam.org/activity/cse/">https://archive.siam.org/activity/cse/</a>. Another example is that SIAG officers regularly get questions about how to engage a SIAG based on the instructions

at <a href="https://archive.siam.org/activity/listservs.php">https://archive.siam.org/activity/listservs.php</a>, which are popularly indexed and do not indicate that SIAM has moved SIAG engagement away from this mode.

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# 8) How can the activity group help SIAM in its general role of promoting computational science and engineering?

SIAG CSE intersects several topics of different SIAGs. CSE practitioners leverage linear algebra, uncertainty quantification, optimization, discrete mathematics and algorithms, data science and supercomputing, and inverse/imaging problems to solve physics-based application problems. SIAG CSE enables experts from these many areas to come together to share research and software and build new collaborations that promote scientific discovery. Its focus on computation advances deploying mathematical research into software tools that run on the most powerful computers in the world. As computer architectures become more complex, the software, algorithms, and expertise of SIAG CSE researchers will play an increasingly important role in mathematics, science and engineering.

The CSE conferences are large and multi-faceted, providing researchers both a broader view of current capabilities and challenges, and greater opportunities to connect with experts across the spectrum of scientific computation. SIAG CSE is eager to expand these opportunities globally, starting with CSE23 in Europe and to continue to innovate at CSE25 and beyond.

This SIAG requests that the SIAM Council and Board of Trustees renew its charter for a two-year operating period beginning January 1, 2023.

Signed, Stefan Wild April 30, 2022